THEOCHEM, VOLUME 38 (1987)

(Journal of Molecular Structure, Vol. 153)

AUTHOR INDEX

Asai, Y. 295

Balázs, A. 103
Bernholdt, D. E. 175
Bock, C. W. 363
Burshtein, K. Ya. 195, 203, 209
Butt, G. 141

Castro, E. A. 215
Chandra, A. K. 357
Clack, D. W. 323
Clark, M. 67
Coussens, B. 227
Craw, J. S. 335

De Maré, G. R. 341
Dogimont, C. 249
Dykstra, C. E. 175

Eckert-Maksić, M. 121, 133
El-Issa, B. D. 241
Epiotis, N. D. 1
Ewbank, J. D. 165

Fukui, K. 295

George, P. 363
Gynther, J. 307

Hankó-Novák, K. 59
Hendrickx, M. 227
Herndon, W. C. 75
Hinchliffe, A. 335
Hori, K. 295

Ikuta, S. 269
Imamura, M. 269
Irwin, J. D. 175
Ivanov, P. M. 147

Jubert, A. H. 215
Jug, K. 221

Kar, T. 93
Kobayashi, S. 295
Konschin, H. 307
Kulkarni, G. V. 357

Lacosse, J. P. 175
Leroy, G. 249
Loushin, S. K. 175

Makhyoun, M. A. 241
Maksić, Z. B. 133
Maksimović, L. 121
Malar, E. J. P. 221
Mälkönen, P. 159
Maluendes, S. A. 215
Mattson, K. J. 175
McKee, M. L. 75
Miers, J. B. 175
Mingdan, C. 323
Mukherjee, D. C. 93

Nagy, P. 59
Neykov, G. D. 147

Orahovats, A. S. 147
Ornellas, F. R. 85

Park, K. D. 175
Peeters, D. 249
Pierloot, K. 227
Pohjala, E. 159

Rouvinen, J. 159, 307

Salsa', B. A. 241
Sana, M. 249
Sannigrahi, A. B. 93
Schaefer, T. 55
Schäfer, L. 165
Sebastian, R. 55
Siam, K. 165
Sletten, E. 289
Stögård, Å. 289
Stradella, O. G. 215
Szász, G. 59

Tachibana, A. 295
Taft, R. W. 141
Tanaka, L. K. 175
Taniguchi, H. 295
Thrasher, J. S. 67
Topsom, R. D. 141
Trachtman, M. 363
Tylli, H. 307

Van Alsenoy, C. 165
Van Hooydonk, G. 275
Vanquickenborne, L. G. 227
Vepsäläinen, J. 159
Verhulst, J. 227

Warren, K. 323
Wilante, C. 249
Williams, G. R. J. 185, 191

Yamabe, T. 295

THEOCHEM, VOLUME 38 (1987)

(*Journal of Molecular Structure, Vol. 153*)

SUBJECT INDEX

Angular overlap model,
the distance dependence of the parameters of the angular overlap model 323
Aromatic and antiaromatic systems,
geometry of triplets and dianions of aromatic and antiaromatic systems 221

Beta-blockers,
structural studies on beta-blockers. Part I. Structural similarities of pronethalol and propranolol 159

C_{60} isomers,
calculated properties of C_{60} isomers and fragments 75
Carbocation,
theoretical study on carbocation with a triple bond 295
Carbon—hydrogen bonding,
inter-relationships between the geometrical parameters for the carbon—hydrogen bonding in the ring in monosubstituted and *para*-disubstituted benzene derivatives: A molecular orbital study 363
CF_3N=CHF,
an ab initio study of the possible isomers and conformations of N-(trifluoromethyl) fluoro methanimine, CF_3N=CHF 67
$[(CH_3)_3C]_2X$
ab initio studies of structural features not easily amenable to experiment. Part 58. Comparison of the molecular structures of some di-tertiarybutyl compounds of type $[(CH_3)_3C]_2X$ 165
Cis-N-Methylformamide,
a comparative ab initio study of amides. Part II. Force fields and vibrational assignments for *N*-methylacetamide and *cis-N*-methylformamide 103
Constrained variational method,
the constrained variational method 335
Cu^+ complexes,
ab initio calculations of Li^+ and Cu^+ complexes of imidazole 289
1,6-Cyclodecadiene systems,
molecular mechanics and quantum-chemical studies of some 1,6-cyclodecadiene systems 147

9,10-Dihydro-anthracene,
some molecular orbital computations of the inversion barrier in 9,10-dihydroanthracene 55
Di-tertiarybutyl compounds,
ab initio studies of structural features not easily amenable to experiment. Part 58. Comparison of the molecular structures of some di-tertiarybutyl compounds of type $[(CH_3)_3C]_2X$ 165

Euclid,
Euclid's golden number and particle interactions 275

Harman,
the molecular structure of norharman and harman: an STO-3G molecular orbital investigation 307
$H_4C_2N_2$ isomers
the structures and stabilities of $H_4C_2N_2$ isomers 175
Heterocycles,
semiempirical quantum-chemical calculations on the protonation of some N-bridgehead heterocycles 59
Heterocyclic molecules,
semiempirical vs. ab initio calculations of molecular properties. Part 4. Nuclear quadrupole coupling constants of ^{14}N in some medium sized heterocyclic molecules 133
H_2PPF_2,
phosphinodifluorophosphine (H_2PPF_2): is there a stable gauche conformer? An ab initio study 85

Imidazole,
ab initio calculations of Li^+ and Cu^+ complexes of imidazole 289
Isopropenylcyclopropane,
ab initio study of conformational behaviour of isopropenylcyclopropane 341

Li^+ complexes,
ab initio calculations of Li^+ and Cu^+ complexes of imidazole 289

N-Methylacetamide,
a comparative ab initio study of amides. Part II. Force fields and vibrational assignments for *N*-methylacetamide and *cis*-*N*-methylformamide 103
MNDO and MNDO/H calculations,
MO studies of solvation effects. Part I. A simple model of solvation for MNDO and MNDO/H calculations 195
MO studies of solvation effects,
MO studies of solvation effects. Part I. A simple model of solvation for MNDO and MNDO/H calculations 195
MO studies of solvation effects. Part II. Influence of solvation on the proton transfer process $NH_3 + HF \rightarrow NH_4^+ + F^-$ 203
MO studies of solvation effects. Part III. S_N2 reactions in the gas phase and in solution 209
Monosubstituted benzene derivatives,
inter-relationships between the geometrical parameters for the carbon—hydrogen bonding in the ring in monosubstituted and *para*-disubstituted benzene derivatives: A molecular orbital study 363
Mulliken and Löwdin SCF density matrices,
comparison of atomic charges, valencies and bond orders in some hydrogen-bonded complexes calculated from Mulliken and Löwdin SCF density matrices 93

N-Bridgehead heterocycles,
semiempirical quantum-chemical calculations on the protonation of some N-bridgehead heterocycles 59
$NH_3 + HF \rightarrow NH_4^+ + F^-$,
MO studies of solvation effects. Part II. Influence of solvation on the proton transfer process $NH_3 + HF \rightarrow NH_4^+ + F^-$ 203
$NH_3 \cdot\cdot X_2$ complexes,
ab initio studies of $NH_3 \cdot\cdot X_2$ complexes 357
Nitrogen-centred radicals,
A theoretical investigation of the structure and reactivity of nitrogen-centred radicals 249
Norharman,
the molecular structure of norharman and harman: an STO-3G molecular orbital investigation 307
Nuclear quadrupole coupling constants,
semiempirical vs. ab initio calculations of molecular properties. Part 4. Nuclear quadrupole coupling constants of ^{14}N in some medium sized heterocyclic molecules 133

ONSNO,
a theoretical study of the structure and vibrational spectrum of SNO, SNONO, and ONSNO 215
Organo sulfur—nitrogen ring systems
hyperpolarizability of conjugated organic systems. Part III. Organo sulfur—nitrogen ring systems 191
Organometallic stereochemistry,
beyond symmetry: from organic to main group to organometallic stereochemistry and back 1

Para-disubstituted benzene derivatives,
inter-relationships between the geometrical parameters for the carbon—hydrogen bonding in the ring in monosubstituted and *para*-disubstituted benzene derivatives: A molecular orbital study 363
Phosphinodifluorophosphine,
phosphinodifluorophosphine (H_2PPF_2): is there a stable *gauche* conformer? An ab initio study 85
Polydiacetylene (polyenyne) oligomers
hyperpolarizability of conjugated organic systems II: polydiacetylene (polyenyne) oligomers 185
Pronethalol
structural studies on beta-blockers. Part I. Structural similarities of pronethalol and propranolol 159
Propranolol
structural studies on beta-blockers. Part I. Structural similarities of pronethalol and propranolol 159

S_N2 reactions,
MO studies of solvation effects. Part III. S_N2 reactions in the gas phase and in solution 209
SNO,
a theoretical study of the structure and vibrational spectrum of SNO, SNONO, and ONSNO 215
SNONO,
a theoretical study of the structure and vibrational spectrum of SNO, SNONO, and ONSNO 215
3- and 4-Substituted pyridinium ions,
acidities of 3- and 4-substituted pyridinium ions 141
3-Substituted tetronic acids,
semiempirical MNDO study of the tautomerism in 3-substituted tetronic acids 121
Th and Ni,
A molecular orbital study of the bonding between Th and Ni in a novel compound 241
Transition metal complexes,
on balanced basis sets in ab initio calculations of transition metal complexes 227
N-(Trifluoromethyl)fluoro methanimine,
an ab initio study of the possible isomers and conformations of *N*-(trifluoromethyl)fluoro methanimine, $CF_3N{=}CHF$ 67
Tritiated water,
ab initio MO study on the β^- decay of tritiated water (OHT) 269